MetabolitePilot™ Software
Streamlined data analysis and interpretation

ONE TOUCH PRODUCTIVITY
In the drug discovery environment, comprehensive metabolite identification is critical. Achieving rapid structural identification and complete characterization of major and low-level metabolites is essential in deciding to push through or fail drug candidates, confidently and quickly.

MetabolitePilot™ Software can streamline the data analysis and interpretation of accurate mass metabolism data by eliminating the bottlenecks classically associated with data review and correlation analysis.

Identify metabolites from accurate mass data fast and efficiently, with a workspace that supports confident decision-making.

- Process and interrogate accurate mass metabolism data
- Employ multiple mass defect filtering for cleaner, more relevant data
- Store and retrieve project data with compound library and results database
- Accelerate data processing and reporting with integrated MS/MS fragment interpretation
- Increase confidence in your results with intelligent scoring and easy-to-visualize color-coding
- Predict formulae with a high level of chemical intelligence
- Quickly visualize kinetic trends with integrated inter-sample correlation features
MetabolitePilot™ Software supports accurate metabolite identification with the AB SCIEX TripleTOF™ 5600 LC/MS/MS System.

- Store parent drug information in compound library
- Batch process multiple sample sets
- Quickly review the results with confidence scoring and color-coding
- Sort the potential candidate list with multiple filtering capabilities
- Increase confidence in MS assignments by correlating analog data
- Store information on found metabolites, including confidence scores, assignments and MS/MS spectra in the results database
- Leverage MS/MS fragment interpretation for integrated structural elucidation
- Accelerate inter-species comparisons or time course studies with integrated sample correlation (applicable to analog data as well)
Accelerate your workflow

From structural elucidation and cross correlation to kinetic trends and reporting

MetabolitePilot™ Software supports the faster and more sensitive intelligent acquisition workflows of the new TripleTOF™ 5600 LC/MS/MS system, an accurate, high-resolution mass platform for definitive metabolite detection.

- SmartSpeed™ Acquisition with up to 100 MS/MS per second
- High resolution at unparalleled speed
- EasyMass™ accuracy without continuous recalibration
- Dynamic background subtraction for increased IDA efficiency
- Real time multiple mass defect filtering for MS/MS
- Neutral loss information dependent acquisition

Up to 30 sample sets can be processed together in a batch, which means multiple project results can be obtained with walk-away convenience.

MetabolitePilot Software finds metabolites through a combination of powerful peak finding algorithms. The most appropriate processing parameters are automatically determined for the selected compound, making it easy to get started.

The combined technological advancements of the TripleTOF 5600 System and MetabolitePilot offer an advanced integrated metabolite identification solution which streamlines accurate and reliable metabolite identification.

MetabolitePilot Software is structured around two simple workspaces: processing and results.

Once the data have been acquired, information about the drug of interest can be stored in MetabolitePilot’s compound library as a first step to the processing workflow and overall storage of project information. The newly integrated MS/MS structural elucidation component provides the ability to perform structural elucidation within the MetabolitePilot Software environment, eliminating the need for additional software packages.

The new integrated correlation functionality allows for cross comparisons of multiple samples over a time course or inter-species comparisons using both MS or analog data.

Batch processing for up to 30 sample sets with walk-away convenience and the flexibility of individual processing parameters for each sample

Multiple peak finding algorithms and confirmation scoring for enhanced confidence in proposed metabolites
MetabolitePilot™, more than just software

MetabolitePilot is a vehicle which accelerates the processing and interpretation of metabolism data. Together with the technology advancements of the TripleTOF™ 5600 System, MetabolitePilot addresses the data processing and interpretation bottleneck of traditional metabolite identification strategies on a range of factors, including:
- Multiple parallel peak finding strategy
- Structure driven parameters

The advanced interpretation functions for structural elucidation streamlines metabolite identification into an industrialized process. First the parent structure is automatically loaded and a theoretical fragmentation of the molecule is performed. The fragments are then correlated with the actual HR-MS/MS spectrum in the acquired data.

Next, MetabolitePilot interprets the fragments to verify if the proposed structure is consistent with MS/MS data. Lastly, the accepted structure and interpretation data are integrated into the Results table and the entire MS/MS fragment interpretation is saved to the results table.

By integrating structural elucidation directly in the software, the data processing, interpretation and reporting are streamlined for faster and more efficient data analysis.

Once the processing is complete, you can review the results in the results workspace, where you’re provided with a confirmation score, so you can easily determine if a peak is a metabolite. Here, the multi-sample correlation functionality allows the user to easily perform a correlation analysis of metabolites across multiple samples, automatically generate plots, overlay analog chromatograms, MS and MS/MS data from multiple samples and species all within a single integrated workspace.

Finally, the results database stores all the important information on the project you’re working on, including, found metabolites, assignments and MS/MS spectra.

- Integrated MS/MS interpretation for structural elucidation
- Integrated inter-sample correlation

Integrated MS/MS fragment interpretation workspace for a more streamlined and efficient data analysis

Correlate the results: The correlation workspace provides a simple and clear view of kinetic trends and relative concentrations and allows the user to quickly visualize disproportionate metabolites across a multi-species comparison within MetabolitePilot.
You invest in our technology. We invest in your success.

As the world leader in mass spectrometry, AB SCIEX solutions are backed by the industry’s most extensive service and support organization. With a network of service professionals, experienced compliance specialists, and over 150 PhD application scientists worldwide, we are dedicated to supporting your technical needs and helping you get the most out of your AB SCIEX systems.

AB SCIEX service professionals are recognized as the most highly qualified in the industry. They are certified on our instrument platforms through a rigorous 4-step certification program, with re-certification occurring every two years. This award-winning program helps to ensure that you receive the most efficient, highest-quality, and most up-to-date service available for AB SCIEX products and technology. Choose from flexible service plans and a variety of services for the right level of support for your laboratory’s needs and budget.

Our customer support network is available to provide expert assistance in the use and application of AB SCIEX products through a comprehensive range of services, including application support, technical service, and training.

Whether you access our service and support team by phone, email, on-site visits, or through our innovative remote monitoring technology, you can be confident that the AB SCIEX organization will be there for you.

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